# Serbian Biochemical Society
# Ninth Conference

with international participation

University of Belgrade – Kolarac Endowment
14-16.11.2019. Belgrade, Serbia

***"Diversity in Biochemistry"***

# Serbian Biochemical Society

**President:** Marija Gavrović-Jankulović
**Vice-president:** Suzana Jovanović-Šanta
**General Secretary:** Milan Nikolić
**Treasurer:** Milica Popović

**Organizing committee**

Natalija Polović
Milan Nikolić
Milica Popović
Karla Ilić Đurđić
Dragana Robajac
Romana Masnikosa
Nataša Simin
Aleksandra Stefanović
Jelena Brkljačić
Isidora Protić-Rosić
Ana Simović
Snežana Spasić
Vladimir Mihailović
Ana Miltojević
Srđan Miletić

**Scientific committee**

Marija Gavrović-Jankulović
Mihajlo B. Spasić
Vesna Niketić
Ivan Spasojević
Dejana Mokranjac
Neda Mimica-Dukić
Snežana Đorđević
Suzana Jovanović-Šanta
Melita Vidaković
Snežana Marković
Olgica Nedić
Ivanka Karadžić
Vesna Spasojević-Kalimanovska
Tanja Ćirković Veličković
Ivan Gržetić
Goran Brajušković
Vesna Vučić
Niko Radulović

## Proceedings

**Editor:** Ivan Spasojević
**Cover design:** Zoran Beloševac
**Publisher:** Faculty of Chemistry, Serbian Biochemical Society
**Printed by:** Colorgrafx, Belgrade

# Anion-π interactions in phycocyanin interfaces: a computational analysis

**Luka M. Breberina[1*], Srđan Đ. Stojanović[2], Milan R. Nikolić[1]**

[1]*Department of Biochemistry, Faculty of Chemistry, University of Belgrade, Belgrade, Serbia*
[2] *Department of Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade*

[*]*e-mail: creativeluani@gmail.com*

We investigated 321 possible anion-π interactions in a data set consisting of different subunit interfaces in 20 phycocyanins PDB structures. We observed that phycocyanobilin tetrapyrrole chromophore is capable of forming anion-π interactions only as an anion. It was found that Tyr is the most common aromatic donor. Although presented in the examined set of interfaces, Trp does not take part in anion-π interactions. Asp-Tyr is the most common anion-π pair, while Glu-His pair does not exist in our data set. Distance examination revealed that anion-π interactions between amino acid residues appear in the range of 3-7 Å, with the average value around 5 Å. The angle between carboxylate and aromatic ring points preference toward higher values, with a peak at 90° and average value around 66°. Interestingly, much less represented anion-π contacts including chromophore show higher values of distance and lower values of this angle. *Ab initio* calculations revealed that interaction energies lay in the range from +0.3 to –14 kcal $mol^{-1}$, with generally much higher values for anion-π interaction pairs between amino acid residues compared to the chromophore including interactions. The most common (>50%) anion-π residue in the stabilization protein centers is Phe, while Glu and His are not presented at all. Anion-π interacting residues have high average conservation score of 7.7, which is especially pronounced for anion residues. The highest conservation score is observed for Asp and the lowest for Phe. Anion-π interacting residues show a preference for buried regions. Almost half of the residues involved in anion-π interactions are also part of hot-spot regions, but only Asp, Phe, and Tyr. Further, in approximately one-fifth of anion-π interaction pairs, both of the residues come from the same hot-spot region and these are exclusively Asp-Tyr contacts. To conclude, a high percentage of anion-π interacting pairs in stabilization centers, their high presence in hot-spot regions and high conservation score, together with the favorable energy profile, imply that these interactions might have a significant role in the stability of phycocyanin oligomers.

## Acknowledgments

This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grants Nos. 172001, 172035).